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Modeling of Particle Behavior in a Wurster Fluidized Bed: Coupling CFD-DEM with Monte Carlo

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Abstract

CFD-DEM approach is applied to investigate circulation motion of particles in a mono-disperse system under both dry and wetting conditions. Good agreement between simulation results and measurement data is observed, in terms of cycle time and residence time in dry condition. The deposition of droplets on the particle surface is modeled by a Monte Carlo approach. The influence of cohesion forces on the macroscopic particle circulation is discussed. In addition, information about coating coverage, the layer thickness and particle size distribution can be predicted by this integrating approach.

***Keywords:** CFD-DEM; Wurster coater; Monte Carlo; cohesion force; residence time.*

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1. Introduction

Particle coating is widely applied in pharmaceutical, food and fertilizer industry. The Wurster coater can be used as a batch or a continuous fluidized bed to precisely control the quality of the coated product [1]. The entire coating process is considerably complex, caused by a large number of sub-processes, including wetting, drying and film formation; and by the presence of different zones with different controlling parameters (such as gas velocity, gas temperature, and spray rate), as shown in Fig. 1. The enhanced understanding of particle dynamics in different zones is significant to optimize drying kinetics that governs particle formation in coating.

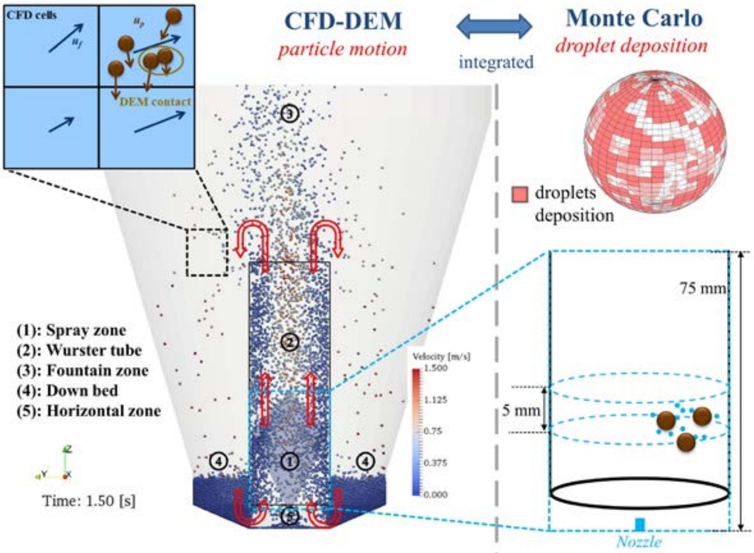

Fig. 1 Modeling of particle behavior by CFD-DEM for particle motion integrating Monte Carlo for droplet deposition (The Wurster coater is divided into 5 process zones; and the droplet deposition takes place in the region marked by the light blue rectangle).

The circulation motion of particles under dry conditions has been investigated in experiments and simulations [2, 3]. However, published studies of the influence of cohesion forces existing in spray zone on the circulation motion are very limited. In this study, computational fluid dynamics-discrete element method (CFD-DEM) was used to investigate the particle motion in the Wurster coater, under both dry and wetting conditions. The influence of cohesion forces, relating to wetting properties and process parameters, on the residence time and the cycle time are discussed based on the analysis of all individual particle trajectories. For the prediction of particle size, a two-zone population balance modeling is usually used to predict the growth of particles during the coating process. In this work, the event of droplet deposition modeled by a Monte Carlo approach [4] was integrated with the particle motion predicted by the CFD-DEM approach, which creates a relatively cost-effective multiscale numerical method to predict particle size distribution and coating coverage during the coating process. The effect of cohesion forces in the Wurster tube on particle size distributions for different process times is discussed.

2. Methodology

2.1 CFD-DEM approach

The CFD-DEM approach has been widely applied to investigate the complex granular flow in chemical applications. The CFD-DEM approach can capture the macroscopic particle dynamics in the multiphase flow, simultaneously providing an insight into behavior of individual particle scale including particle-particle interactions, as shown in Fig. 1. The open source code OpenFoam+LiGGGHTS (CFDEM®project) was used for this study. The detailed governing equations of solid and gas phase, Gidaspow drag model, Hertz soft sphere contact model and rolling model can be found in our previous works [3, 5].

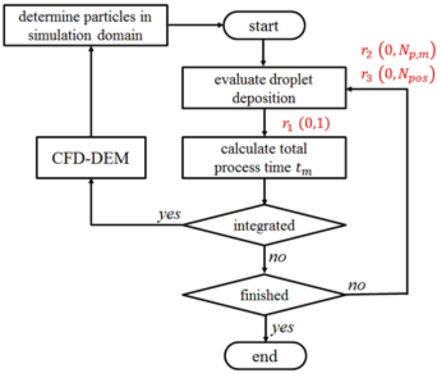

Fig. 2 Flow chart of the Monte Carlo integrated with CFD-DEM including required random numbers ($N_{p,m}$ is the number of particles in the Monte Carlo domain).

2.2 Cohesion model

The capillary force and viscosity force have been implemented into the DEM code [6]. The equation for calculating the capillary force F_c (N) of a specific particle-pair geometry was obtained by fitting the set of discrete solutions of the Laplace equation, expressed as:

$$F_c = \pi\sigma\sqrt{R_i R_j}\left[C + exp\left(A\frac{d_{inter}}{\max(R_i, R_j)} + B\right)\right], \tag{1}$$

where R_i and R_j are radii of two particles (m), d_{inter} is the inter-particle distance (m), and σ is the surface tension of lqiud (N/m). The coefficients A, B and C are functions of liquid volume V_l (m^3), contact angle θ (radians) and larger particle radius $R_{max} = max(R_i, R_j)$ [6]. The liquid volume between two particles is assumed to be evenly distributed when the inter-particle distance is larger than the rupture distance $D_r = (1 + 0.5\theta) \cdot V_l^{1/3}$ (m).

The viscosity force F_v (N) can be calculated as:

$$F_{v,n} = 6\pi\mu R^* v_n \frac{R^*}{d_{inter}}, \qquad F_{v,t} = 6\pi\mu R^* v_t \left[\frac{8}{15} ln \frac{R^*}{d_{inter}} + 0.9588\right], \tag{2}$$

where μ is the fluid dynamic viscosity (Pa·s), $R^* = R_i R_j/(R_i + R_j)$ is the equivalent radius; and v_n and v_t are relative velocity of two particles in normal and tangential directions (m/s), respectively. The capillary force and viscosity force are included into Newton's law of motion for individual particle. Note that these two forces only exist in the Wurster tube and wall boundaries are assumed in dry condition.

2.3 Monte Carlo approach

According to the geometry of spray zone, the simulation domain for Monte Carlo is the cylinder with the height of 75 mm and the radius of the Wurster tube, and the bottom of the domain is aligned with the tip of the spray nozzle, as shown in Fig. 1. The particles in the Monte Carlo domain were determined by the CFD-DEM data. The overview of the Monte Carlo integrated with CFD-DEM is given in Fig. 2. In each Monte Carlo time step Δt_m, one droplet deposition event is guaranteed to happen in the Monte Carlo domain. The time step can be calculated from the number flow rate of droplets injecting into the system, expressed as:

$$\Delta t_m = -(\frac{6\dot{M}}{\pi\rho_d d_d^3})^{-1} \ln r_1, \tag{3}$$

where $\dot{M}$ is the mass flow rate of solution and r_1 is a uniformly distributed random number for the interval (0,1). The droplet diameter is constant. Once the total Monte Carlo process time t_m exceeds 0.01 s, CFD-DEM simulation was advanced for 0.01 s and number of particles in the Monte Carlo domain $N_{p,m}$ was updated based on new CFD-DEM data.

To evaluate the individual droplet deposition, two more random numbers are required: r_2 to pick up the particle from the domain and r_3 to choose deposition position on the single particle surface. In current work, each particle in the domain has the same possibility to receive the droplets. Based on the work of Rieck et al. [4], the number of positions (with same size) per particle N_{pos} is calculated by $N_{pos} = d_p^2/d_{contact}^2$. The diameter d_{contat} is the diameter of contact area, which depends on the contact angle and droplet volume. N_{pos} was rounded to an integer value in the code. Each position can have four statuses labeled by four numbers in the model: 1) no droplet (initial), 2) with wetting droplet, 3) with dry droplet and 4) no droplet (new). In cases of label 1, 3 and 4, the droplet deposition event can occur. If a wetted position (2) is selected, a new random number r_3 is generated until the requirement of deposition is satisfied.

The criterion for determining dry or wet position is related to the drying process of the deposited droplet, expressed as:

Table 1. Summary of the setup for CFD-DEM integrating with Monte Carlo

Parameters	**Value**	**Unit**
Particle phase (DEM)		
Particle diameter $d_{p,0}$	1.75	mm
Particle density ρ_d	1420	kg/m^3
Particle number	50 000	-
Gas phase (CFD)		
Gas density ρ_g	1.2	kg/m^3
Dynamic viscosity	1.84×10^{-5}	Pa·s
Gas flow rate (fluidization $\dot{V}_g$/atomization)	80.3/3.5	m^3/h
Gas temperature	50	^{o}C
Moisture content of fluidization gas Y_{inlet}	1	g/kg
Liquid phase (Monte Carlo)		
Droplet diameter d_d	50	µm
Droplet density ρ_d	1000	kg/m^3
Solid density of coating solution ρ_s	1000	kg/m^3
Mass flow rate $\dot{M}$	0.25	kg/h
Solid mass fraction ϵ_s	0.3	-
Porosity of coating layer φ_s	0.5	-
Liquid content α_l	0.001	-
Surface tension σ	0.072	N/m
Contact angle θ	30	°
Liquid viscosity μ	10^{-4}	Pa·s
CFD-DEM simulation parameters		
CFD time step	5×10^{-5}	s
CFD cell number (structured hexahedral)	81600	-
DEM time step	10^{-5}	s
Integrate time Monte Carlo and CFD-DEM	0.01	s
Simulation time	20	min

$$t_m \geq t_{deposition} + \Delta t_{drying}, \tag{4}$$

where $t_{deposition}$ is the moment the droplet deposition happens, and Δt_{drying} is the drying time of the deposited droplet. Considering the first drying period only, the Δt_{drying} can be calculated by [4]:

$$\Delta t_{drying} = \frac{\left(\frac{1}{6}\pi d_d^3\right) \cdot \rho_d \cdot (1 - \epsilon_s)}{\beta_m A_{dep} \rho_g (Y_{sat} - Y)}, \tag{5}$$

where β is the mass transfer coefficient (m/s), Y_{sat} is the adiabatic saturation moisture content of fluidization gas (g liquid/kg dry gas), and $Y = Y_{inlet} + \dot{M} \cdot (1 - \epsilon_s)/(\dot{V}_g \cdot \rho_g)$ is the moisture content of bulk gas. A_{dep} is the curved area of deposit droplet in contact with the gas (m^2), which can be calculated by:

$$A_{dep} = \frac{1}{2}\frac{\pi \cdot d_{contact}^2}{1+\cos\theta}. \tag{6}$$

The thickness of solid layer in single position on particle surface h_i can be calculated as:

$$h_i = \left(\frac{d_{core}^3}{8} + \frac{3}{4}\frac{N_{pos} \cdot \left(\frac{1}{6}\pi d_d^3\right) \cdot \frac{\rho_d \cdot \epsilon_s}{\rho_s \cdot \varphi_s}}{\pi}\right)^{1/3} - d_{core}, \tag{7}$$

where d_{core} is the diameter of core particle. The coating coverage Ψ can be evaluated by:

$$\Psi = \frac{N_{pos,tot} - N_{pos,free}}{N_{pos,tot}}, \tag{8}$$

where $N_{pos.tot}$ and $N_{pos.free}$ are total number of positions and number of positions without droplet, respectively. With the average coating thickness h_m, the particle diameter can be expressed as: $d_p = d_{core} + 2h_m$.

2.4 Simulation setups

The mesh of Wurster coater was built by O-grid method [3], according to the configuration used in PEPT experiments [2]. The initial particle diameter $d_{p,0}$ is 1.75 mm. All important simulation parameters in the sub-models of CFD-DEM integrating with Monte Carlo are summarized in Table 1. The coupling interval between DEM and CFD is 100 time steps of DEM; and the integrating interval with Monte Carlo is 0.01 s, which is approximately $2d_{p,0}/v_m$ (mean particle velocity in the Wurster tube).

3. Results and discussion

3.1 Particle circulation motion

As shown in Fig. 3, the global circulation of particle from simulation with cohesion forces (0.1 %) is very similar to that in dry condition; however, the particles tend to be clustered in the Wurster tube. The detailed value of mean cycle time and mean residence time are listed in Table 2. The ideal cycle time and residence time in the Wurster tube were found to be in good agreement with PEPT measurement data in dry condition. However, the non-ideal cycle was underestimated in the simulation. With the effect of cohesion forces, the ideal cycle time and the fractions of ideal cycle are decreased, resulting in the increase of total cycle time. The decrease of the fractions of ideal cycle may cause by upwards and downwards motion of particle clustering in the Wurster zone.

3.2 Particle coating

Figure 4 left) shows the coating coverage of a sample particle after 70 s and the spherical particle was mapped into 2D space based on number of deposition positions. The gray level

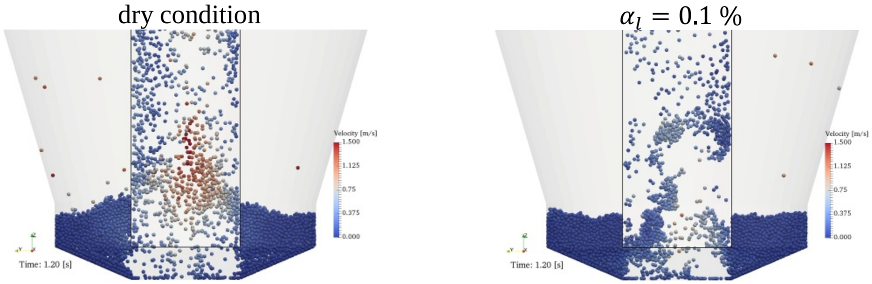

Fig. 3 Influence of cohesion forces on particle motion in the Wurster coater.

Table 2. Comparison of ideal cycle time, overall cycle time, residence time

Variable	**CFD-DEM simulation**		**Measurement** [2]
	dry	$\alpha_l = 0.1\%$	*dry*
$\bar{t}_{ic}$ [s]	4.98 (52.8)	4.25 (33.5)	4.84 (99.0)
$\bar{t}_c$ [s]	5.82 (61.5)	6.42 (73.3)	6.14 (89.8)
r_n [%]	78.3	60.2	55.3
$\bar{t}_{r,t}$ [s]	0.96 (33.7)	0.90 (44.6)	1.00 (-)
$\bar{t}_{r,s}$ [s]	0.15 (22.1)	0.14(28.3)	-

$*\,\bar{t}_{ic}$ is mean ideal cycle time, $\bar{t}_{ic}$ is mean total cycle time, r_n is number ratio of ideal cycle, $\bar{t}_{r,t}$ and $\bar{t}_{r,t}$ are mean residence times in Wurster tube and spray zone; the coefficient of variation (CV) is in the brackets.

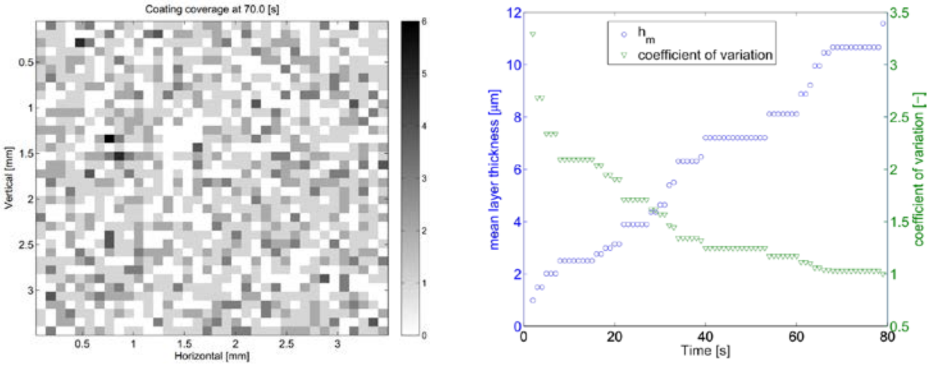

Fig. 4 Coating coverage and layer thickness of sample particle from wetting simulation: left) droplet deposition on single particle, right) layer thickness and CV with respect to time.

represents the number of deposition droplets in each pixel. According to Eq. (8), the coating coverage at this moment is 67 %. However, the coating coverage cannot roundly measure the uniformity of coating layer. The coefficient of variation (the ratio of standard deviation to mean) of the layer thickness is 1.05 at this moment. Figure 4 right) shows that the mean layer thickness increases and the coefficient of variation decreases. The variation only happens when the particle passes through the Wurster tube. Figure 5 show the size distributions under dry and wetting conditions. There are wider distributions of particle diameter d_p for simulations with cohesion forces for different process times.

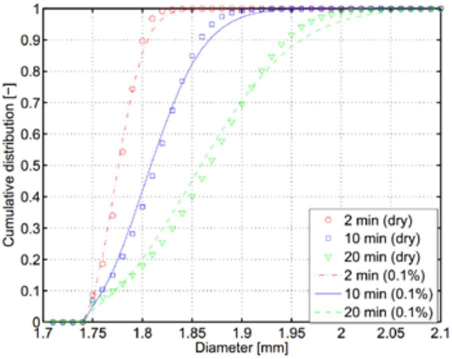

Fig. 5 Particle size distributions of 50000 particles in different process time (both dry and wetting).

4. Conclusion

Cohesion forces scatter distributions of cycle time, residence time and particle size. It is important to provide enough drying capacity in fluidization gas to prevent the appearance of particle agglomeration and achieve high product quality in the Wurster coating process.

5. Acknowledgements

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